Uncertainty Quantification and Reliability Analysis-Based Design Optimization Capabilities in DAKOTA

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Optimization and Uncertainty Quantification
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http://endo.sandia.gov/DAKOTA

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Why Uncertainty Quantification (UQ)?

Need to design systems given <u>uncertain/variable</u> material properties, manufacturing processes, operating conditions, models, measurements…

Uncertainty must be properly modeled to quantify risk and design <u>robust and reliable</u> systems.

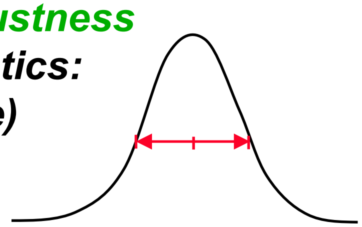
<u>**Aleatory / irreducible**</u> inherent variability with sufficient data (probabilistic models)	vs.	<u>**Epistemic / reducible**</u> uncertainty from lack of knowledge (non-probabilistic models)

Employ a UQ-based approach to optimization under uncertainty (OUU)

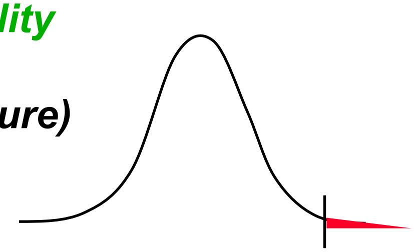
- **safety factors, multiple operating conditions, local sensitivities insufficient**
- **tailor OUU methods to strengths of different UQ approaches**

OUU methods encompass both:

design for robustness
(moment statistics: mean, variance)



design for reliability
(tail statistics: probability of failure)



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Uncertainty-Aware Design

Rather than designing and then post-processing to evaluate uncertainty…

Standard NLP

$$
\begin{array}{ll}
\text{minimize} & f(d) \\
\text{subject to} & g_l \leq g(d) \leq g_u \\
 & h(d) = h_t \\
 & d_l \leq d \leq d_u
\end{array}
$$

…actively design while accounting for uncertainty/reliability metrics

Augment with general response statistics $\mathbf{s_u}$
*(e.g. μ, σ, or reliability **z/β/p**) with linear map*

$$
\begin{array}{ll}
\text{minimize} & f(d) + W s_u(d) \\
\text{subject to} & g_l \leq g(d) \leq g_u \\
 & h(d) = h_t \\
 & d_l \leq d \leq d_u \\
 & a_l \leq A_i \, s_u(d) \leq a_u \\
 & A_e \, s_u(d) = a_t
\end{array}
$$

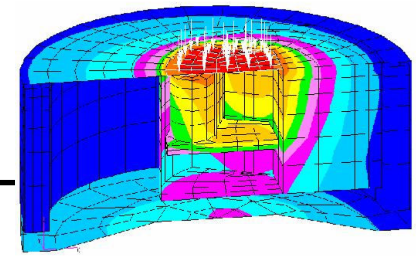
Focus on large-scale simulation-based engineering applications:

- **mostly PDE-based, often transient, some agent-based/discrete event models**
- **response mappings (fns. and constraints) are nonlinear and implicit**

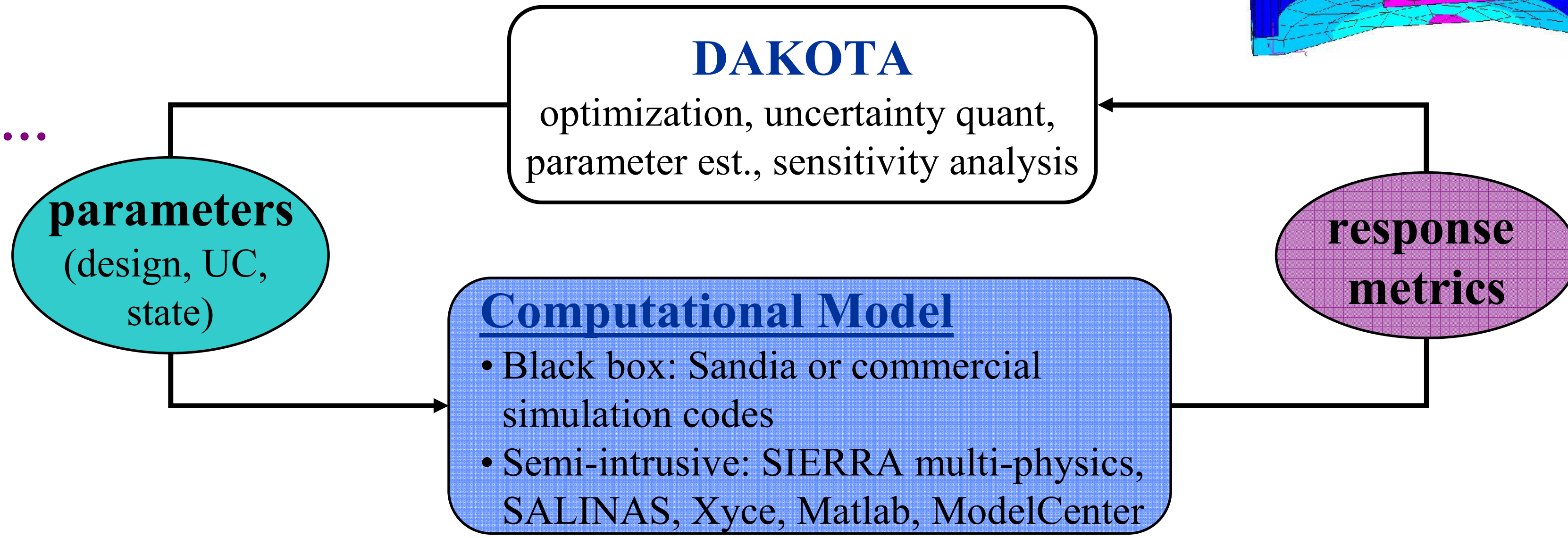
Outline

- Motivation
- DAKOTA toolkit overview
- Uncertainty quantification (UQ) – forward propagation:
  - Sampling-based
  - Reliability analysis
- Enriching optimization with UQ
- Example problem – MEMS
- Conclusion

DAKOTA Overview



iterative analysis…

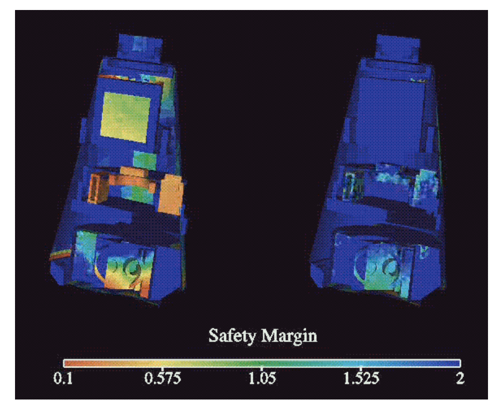


Goal: answer fundamental engineering questions

- What is the best design? How safe is it?
- How much confidence do I have in my answer?

Challenges

- **Software:** reuse tools and common interfaces
- **Algorithm R&D:** nonsmooth/discontinuous/multimodal, mixed variables, unreliable gradients, costly sim. failures
- **Scalable parallelism:** ASCI-scale apps & architectures



Nominal Optimized

Impact: Tool for DOE labs and external partners, broad application deployment, free via GNU GPL (~3000 download registrations)

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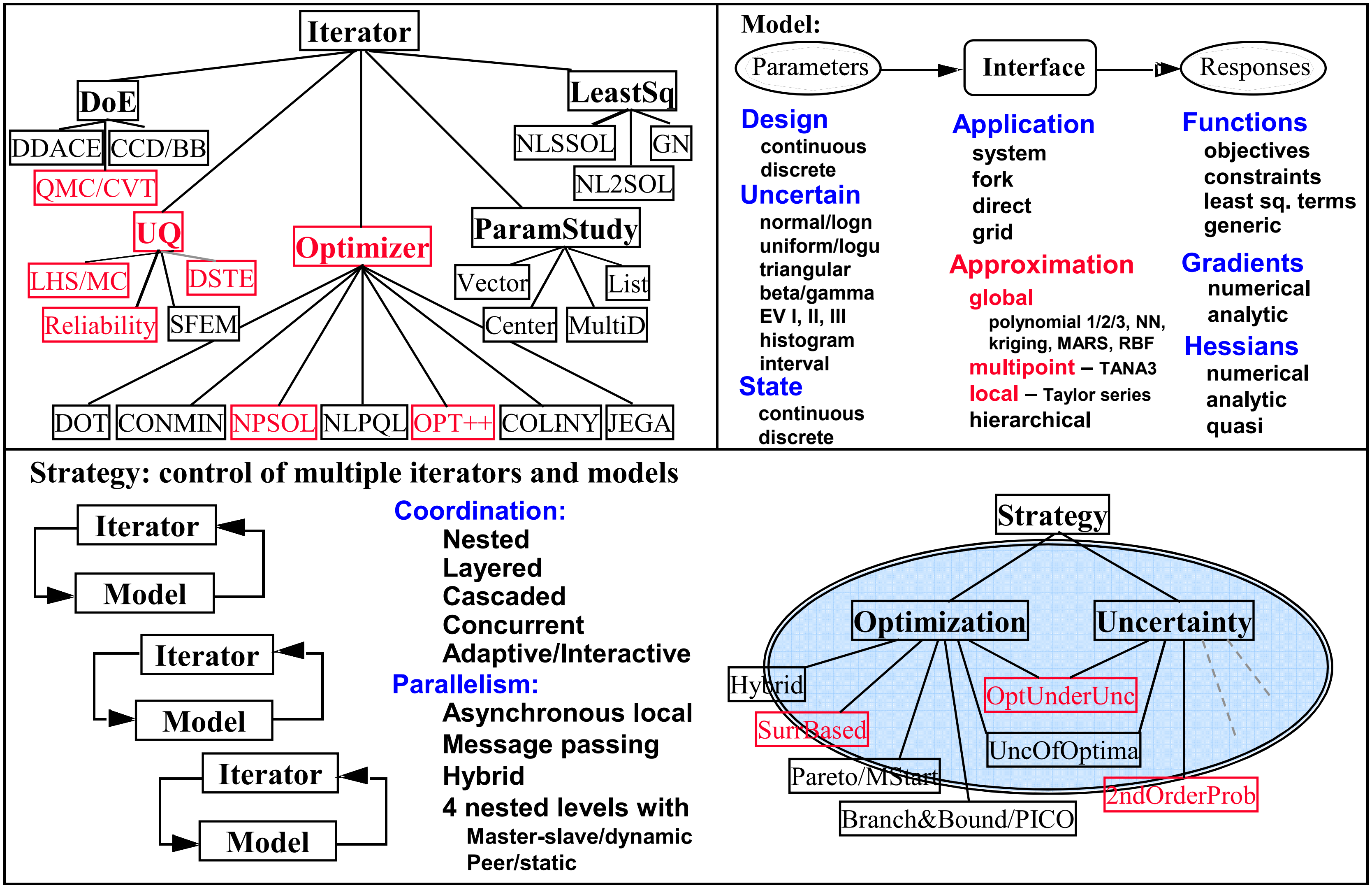
DAKOTA Framework



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Uncertainty Quantification

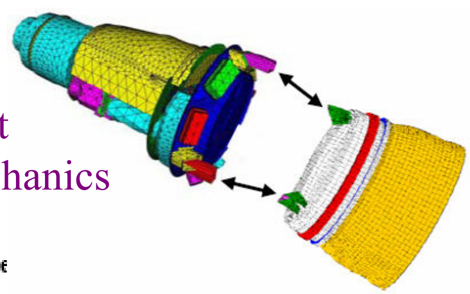
Forward propagation: quantify the effect that uncertain input variables have on model output

Given distributions…

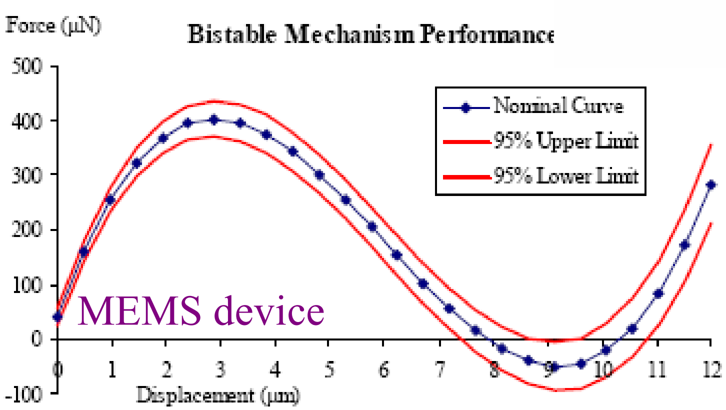
Input Variables → **Computational Model** → **Performance Measures**

GOALS:
- **determine variance of outputs based on uncertain inputs (UQ)**
- **identify inputs whose variances contribute most to output variance (global sensitivity analysis)**

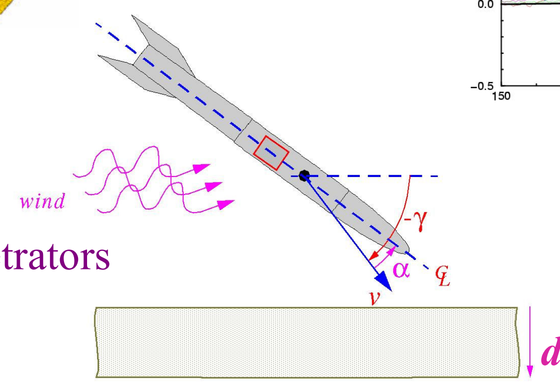
UQ Applications



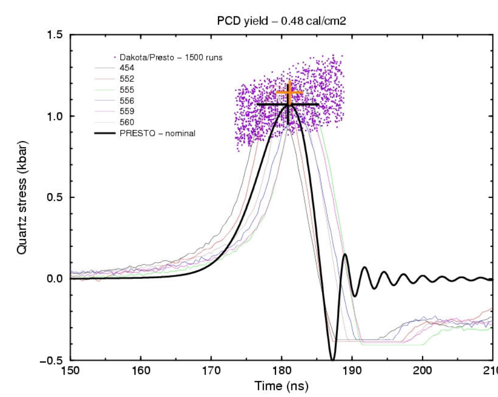
joint mechanics



MEMS device



penetrators



shock physics

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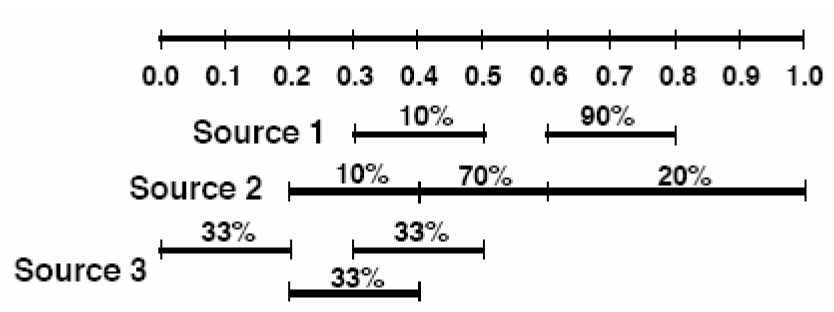
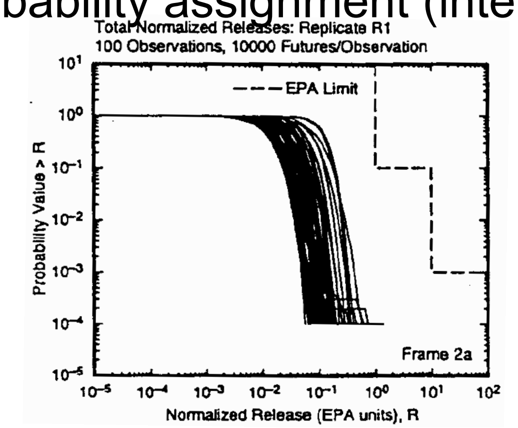
Uncertainty Quantification Methods

Active UQ development in DAKOTA (new, developing, planned)

- **Sampling:** LHS/MC, QMC/CVT, Bootstrap/Importance/Jackknife
  Gunzburger collaboration
- **Reliability:** Evaluate probability of attaining specified outputs / failure
  MVFOSM, x/u AMV, x/u AMV+, FORM (RIA/PMA mappings),
  MVSOSM, x/u AMV^2, x/u AMV^2+, TANA, SORM (RIA/PMA)
  Renaud/Mahadevan collaborations
- **SFE:** Polynomial chaos expansions (quadrature/cubiture extensions).
  Ghanem (Walters) collaborations
- **Metrics:** Importance factors, partial correlations, main effects, and variance-based decomposition.
- **Epistemic:** 2nd-order probability: combines epistemic and aleatory;
  Dempster-Schafer: basic probability assignment (intervals);
  Bayesian





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Sampling Capabilities

Parameter Studies

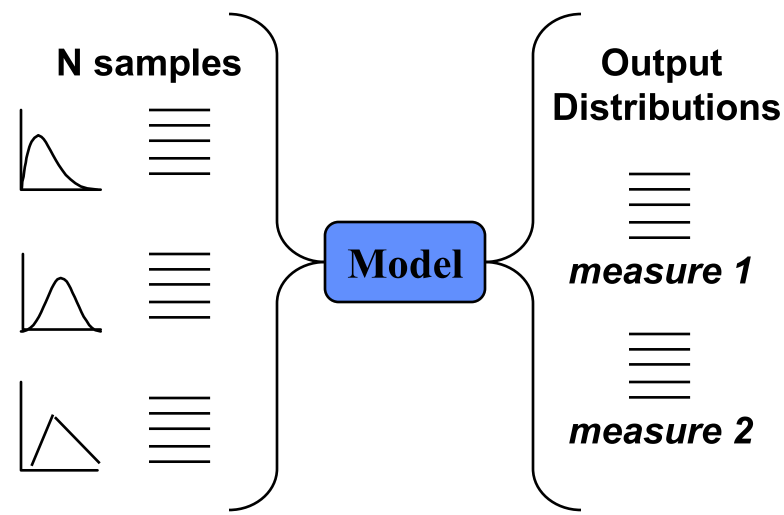
- perturb each variable
- "one-off" or one at a time
- simple but inefficient

Design of Computer Experiments (DACE) and Design of Experiments (DOE)

- Box-Behnken, Central Composite
- factorial and fractional designs
- orthogonal arrays

Sampling Methods – typical for forward UQ propagation

- Standard Monte Carlo
- Pseudo-Monte Carlo: Latin Hypercube Sampling (samples from equi-probability bins for all 1-D projections)
- Quasi-Monte Carlo (low discrepancy): Hammersley, Halton
- Centroidal Voroni Tesselation (CVT): approx. uniform samples over arbitrarily shaped parameter spaces



Also useful for constructing data fit or spanning ROM surrogates.

Analytic Reliability Methods for UQ

- Define limit state function *g(x)* for response metric (model output) of interest, where x are uncertain variables.
- Reliability methods either
  - map specified response levels $g(x) = \bar{z}$ (perhaps corr. to a failure condition) to reliability index ***β*** or probability *p*; or
  - map specified probability or reliability levels to the corresponding response levels.

Mean Value (first order, second moment – MVFOSM)

determine mean and variance of limit state:

$$\begin{aligned}\mu_g &= g(\mu_{\mathbf{x}}) \\ \sigma_g &= \sum_i \sum_j Cov(i,j) \frac{dg}{dx_i}(\mu_{\mathbf{x}}) \frac{dg}{dx_j}(\mu_{\mathbf{x}})\end{aligned}$$

$$\bar{z} \to p, \beta \left\{ \begin{aligned} \beta_{cdf} &= \frac{\mu_g - \bar{z}}{\sigma_g} \\ \beta_{ccdf} &= \frac{\bar{z} - \mu_g}{\sigma_g} \end{aligned} \right. \qquad \bar{p}, \bar{\beta} \to z \left\{ \begin{aligned} z &= \mu_g - \sigma_g \bar{\beta}_{cdf} \\ z &= \mu_g + \sigma_g \bar{\beta}_{ccdf} \end{aligned} \right.$$

simple approximation, but widely used by analysts

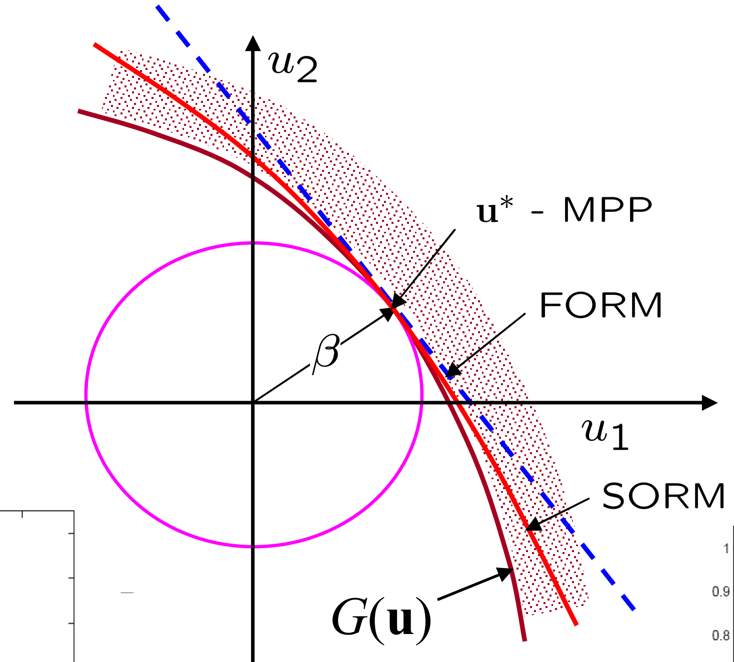
Analytic Reliability: MPP Search

Perform optimization **in u-space (std normal space corr. to uncertain x-space) to determine Most Probable Point (of response or failure occurring)**

Reliability Index Approach (RIA)

$$\text{minimize} \quad \mathbf{u}^T\mathbf{u}$$
$$\text{subject to} \quad G(\mathbf{u}) = \bar{z}$$

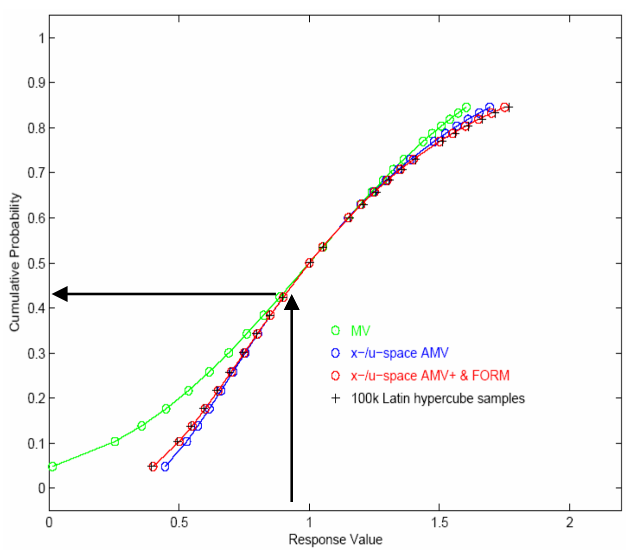
Find min dist to *G* level curve
Used for fwd map *z* → *p/β*



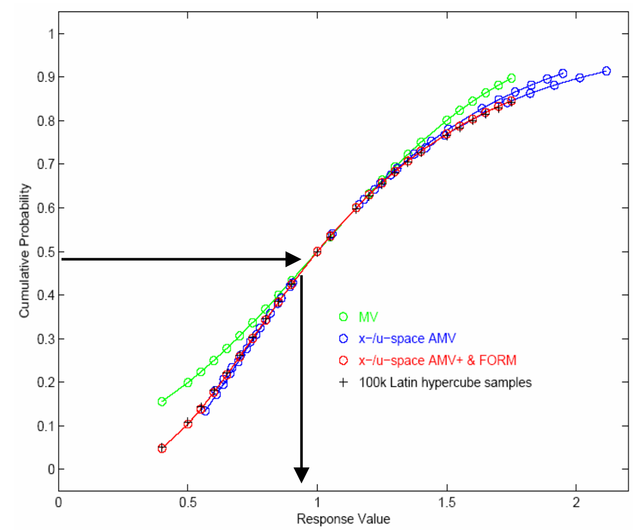
Performance Measure Approach (PMA)

$$\text{minimize} \quad \pm G(\mathbf{u})$$
$$\text{subject to} \quad \mathbf{u}^T\mathbf{u} = \bar{\beta}^2$$

Find min *G* at *β* radius
Better for inv map *p/β* → *z*



...should yield better estimates of reliability than Mean Value methods



Reliability: Algorithmic Variations

Many variations possible to improve efficiency, including in DAKOTA…

- **Limit state linearizations: use a surrogate for the limit state during optimization**

$$\text{AMV:} \quad g(\mathbf{x}) = g(\mu_{\mathbf{x}}) + \nabla_x g(\mu_{\mathbf{x}})^T(\mathbf{x} - \mu_{\mathbf{x}})$$

$$\text{u-space AMV:} \quad G(\mathbf{u}) = G(\mu_{\mathbf{u}}) + \nabla_u G(\mu_{\mathbf{u}})^T(\mathbf{u} - \mu_{\mathbf{u}})$$

$$\boxed{\text{AMV+:} \quad g(\mathbf{x}) = g(\mathbf{x}^*) + \nabla_x g(\mathbf{x}^*)^T(\mathbf{x} - \mathbf{x}^*)}$$

$$\text{u-space AMV+:} \quad G(\mathbf{u}) = G(\mathbf{u}^*) + \nabla_u G(\mathbf{u}^*)^T(\mathbf{u} - \mathbf{u}^*)$$

FORM: no linearization

(also 2nd order approximations – can use full or quasi-Newton Hessians in optimization)

- **Integrations (in u-space to determine probabilities):**

$$1^{st}\text{-order:} \begin{cases} p(g \le z) & = & \Phi(-\beta_{cdf}) \\ p(g > z) & = & \Phi(-\beta_{ccdf}) \end{cases} \qquad 2^{nd}\text{-order:} \begin{cases} p = \Phi(-\beta) \underbrace{\prod_{i=1}^{n-1} \frac{1}{\sqrt{1+\beta\kappa_i}}}_{\text{curvature correction}} \end{cases}$$

- **MPP search algorithm**

  [HL-RF], Sequential Quadratic Prog. (SQP), Nonlinear Interior Point (NIP)

- **Warm starting**

  When: AMV+ iteration increment, $z/p/\beta$ level increment, or design variable change

  What: linearization point & assoc. responses (AMV+) and MPP search initial guess

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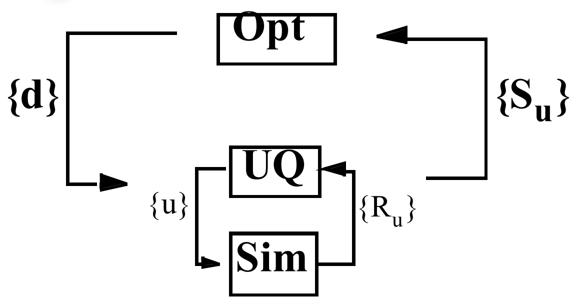
Optimization Under Uncertainty



nested paradigm

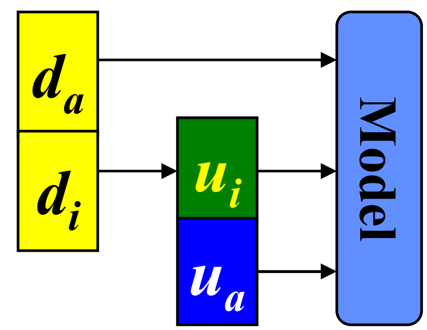
optimize, accounting for uncertainty metrics

(use any of surveyed UQ methods)

$$
\begin{array}{ll}
\min & f(d) + W s_u(d) \\
\text{s.t.} & g_l \le g(d) \le g_u \\
 & h(d) = h_t \\
 & d_l \le d \le d_u \\
 & a_l \le A_i\, s_u(d) \le a_u \\
 & A_e\, s_u(d) = a_t
\end{array}
$$

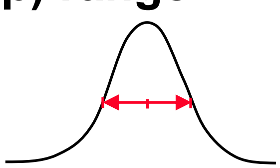
Input design parameterization

- **Uncertain variables augment design variables in simulation**
- **Inserted design variables: an optimization design variable may be a parameter of an uncertain distribution, e.g., design the mean of a normal.**

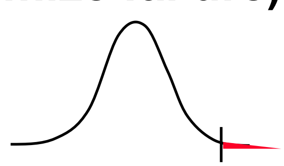


Response metrics

Robustness:
min/constrain σ^2 or G(β) range



Reliability:
max/constrain *p*/β (minimize failure)



Combined/other:
pareto tradeoff, LSQ: model calibration under uncertainty

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Sample of RBDO Algorithms

Bi-level RBDO

- **Constrain RIA $z \rightarrow p/\beta$ result**
- **Constrain PMA $p/\beta \rightarrow z$ result**

RIA RBDO
$$\begin{cases} \text{minimize} & f \\ \text{subject to} & \beta \geq \bar{\beta} \\ \text{or} & p \leq \bar{p} \end{cases}$$

PMA RBDO
$$\begin{cases} \text{minimize} & f \\ \text{subject to} & z \geq \bar{z} \end{cases}$$

Fully analytic Bi-level RBDO

- **When nesting UQ analysis, analytic reliability sensitivities avoid numerical differencing at design level**

$$\begin{cases} \nabla_{\mathbf{d}} z = \nabla_{\mathbf{d}} g \\ \nabla_{\mathbf{d}} \beta_{cdf} = \dfrac{1}{\| \nabla_{\mathbf{u}} G \|} \nabla_{\mathbf{d}} g \\ \nabla_{\mathbf{d}} p_{cdf} = -\phi(-\beta_{cdf}) \nabla_{\mathbf{d}} \beta_{cdf} \end{cases}$$

(1st order)

*If **d** a distribution param., then expand:*

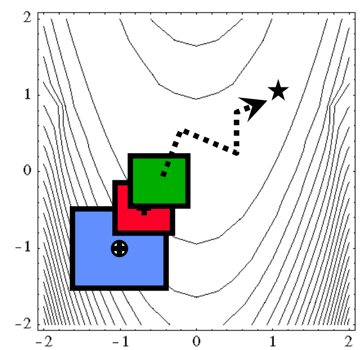
$$\nabla_{\mathbf{d}} g = \nabla_{\mathbf{d}} \mathbf{x} \nabla_{\mathbf{x}} g$$

Sequential/Surrogate-based RBDO:

- **Break nesting: iterate between opt & UQ until target is met. Trust-region surrogate-based approach is non-heuristic.**

$$\begin{array}{ll} \text{minimize} & f(\mathbf{d}_0) + \nabla_d f(\mathbf{d}_0)^T (\mathbf{d} - \mathbf{d}_0) \\ \text{subject to} & \beta(\mathbf{d}_0) + \nabla_d \beta(\mathbf{d}_0)^T (\mathbf{d} - \mathbf{d}_0) \geq \bar{\beta} \\ & \| \mathbf{d} - \mathbf{d}_0 \|_\infty \leq \Delta^k \end{array}$$

1st-order
(also 2nd-order, …)



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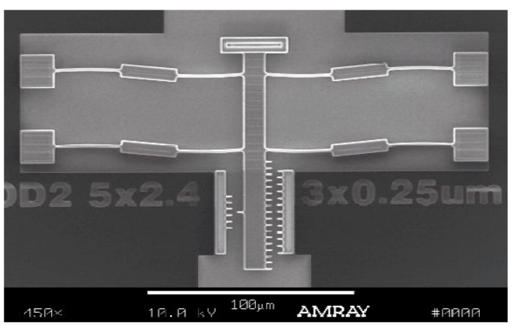
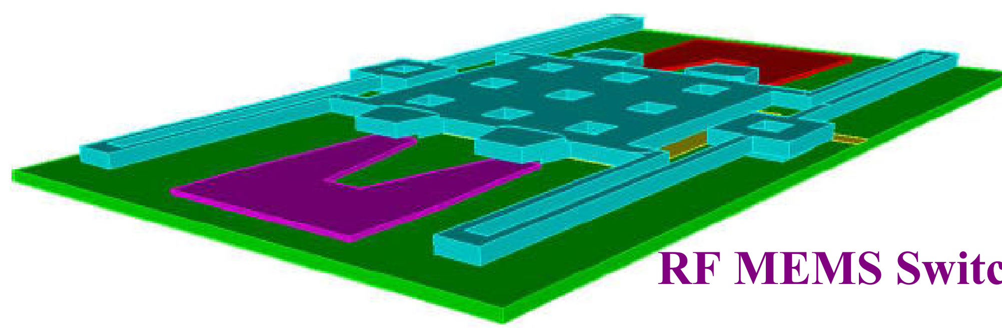
Engineering Application Deployment:
Shape Optimization of Compliant MEMS

- Micro-electromechanical system (MEMS) designs are subject to substantial variabilities and lack historical knowledge base
- Sources of uncertainty:
  - Material properties, manufactured geometries, residual stresses
  - Data can be obtained → aleatoric uncertainty, probabilistic approaches
- Resulting part yields can be low or have poor cycle durability
- Goals: shape optimization to…
  - Achieve prescribed reliability
  - Minimize sensitivity to uncertainties (robustness)
- Nonlinear FE simulations
  - ~20 min. desktop simulation expense (SIERRA codes: Adagio, Aria, Andante)
  - Remeshing during shape design with FASTQ/CUBIT
    or smooth mesh movement with DDRIV
  - (semi-analytic) $p/\beta/z$ gradients appear to be reliable

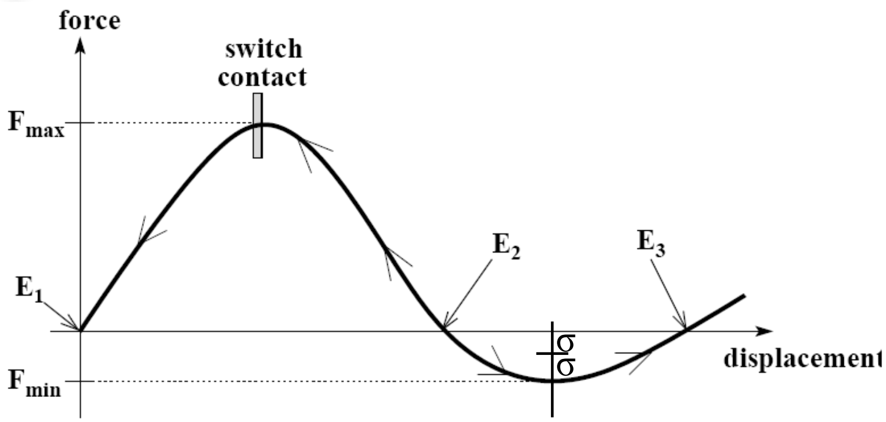


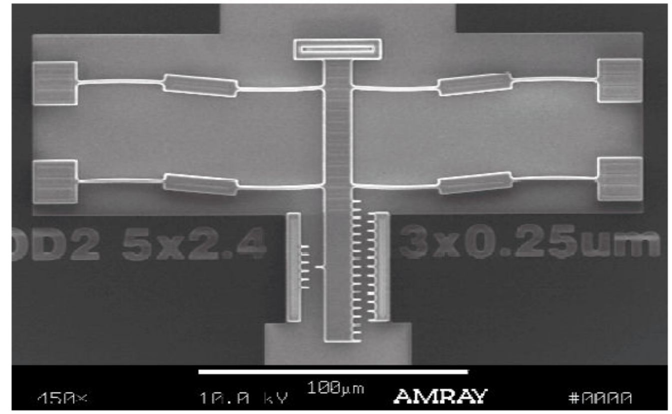
Bi-stable
MEMS Switch



RF MEMS Switch

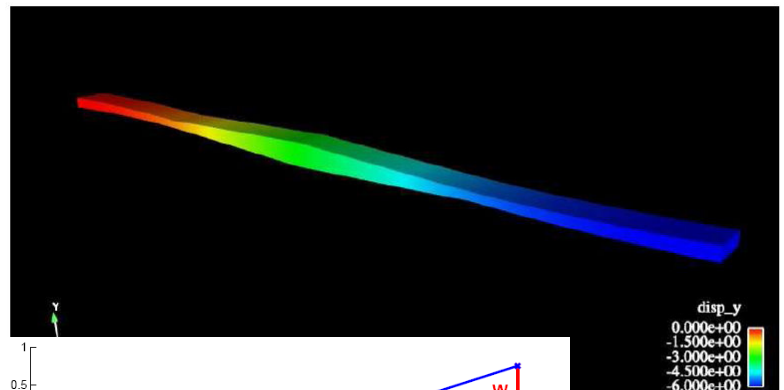
Bi-Stable Switch: Problem Formulation

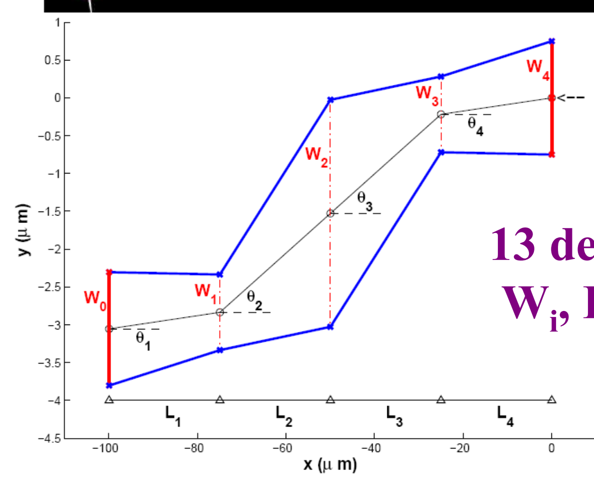




simultaneously reliable AND robust designs

$$
\begin{array}{llcll}
\max & & & F_{min}(\mathbf{d}, \mu) & \\
\text{s.t.} & 2 & \leq & \beta(\mathbf{d}) & \\
 & 50 & \leq & F_{max}(\mathbf{d}, \mu) & \leq 150 \\
 & & & E_2(\mathbf{d}, \mu) & \leq 8 \\
 & & & S_{max}(\mathbf{d}, \mu) & \leq 1200
\end{array}
$$





2 random variables

variable	mean	std. dev.	distribution
Δw	-0.2 μm	0.08	normal
S_r	-11 Mpa	4.13	normal

13 design vars *d*: W_i, L_i, θ_i

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Bi-Stable Switch: Results (DOT/MMFD)

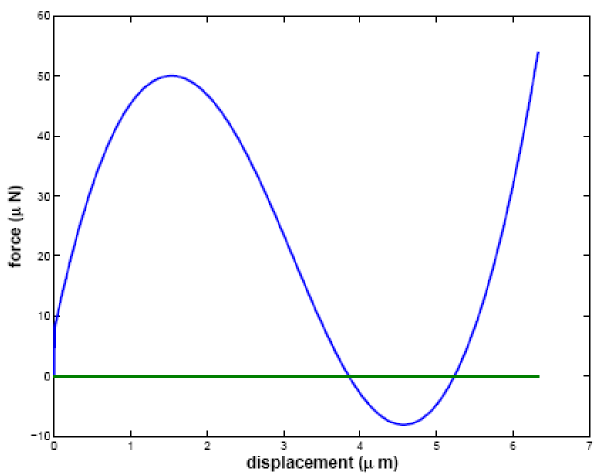
lower bound	RBDO metric	upper bound	MVFOSM initial	MVFOSM optimal	AMV+/FORM initial	AMV+/FORM optimal
	F_{min} (μN)		-23.03	-8.08	-23.03	-9.37
2	β		5.66	$\boxed{2.00}$	4.02	$\boxed{2.00}$
50	F_{max} (μN)	150	67.35	50.0	67.35	50.0
	E_2 (μm)	8	4.06	3.85	4.06	3.76
	S_{max} (MPa)	1200	396	313	396	323
	Verified β		4.02	$\boxed{1.75}$		

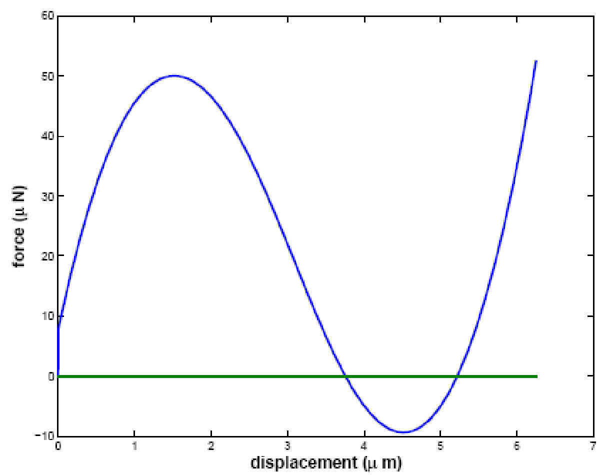
Reliability: target achieved for AMV+/FORM; target approximated for MV

Robustness: variability in F_{min} reduced from 5.7 to 4.6 μN per input σ [$\mu_{F_{min}}/\beta$]

Ongoing: quantity of interest error estimates → error-corrected UQ/RBDO

MVFOSM-based RBDO





AMV+/FORM-based RBDO

Conclusions

- Uncertainty-aware design optimization is helpful in engineering applications where robust and/or reliable designs are essential.
- The DAKOTA toolkit includes algorithms for uncertainty quantification and optimization of computational models .
- DAKOTA strategies enable combination of algorithms, use of surrogates and warm-starting, and leveraging massive parallelism.
- Advanced analytic reliability techniques may offer more refined estimates of uncertainty than sampling or mean value methods and may be more suitable in an optimization context.
- Further UQ and OPT capabilities are in development as is deployment to additional applications.

Thank you for your attention!

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